

# The narrow peak on the frequency dependance of the susceptibility of the harmonical oscillator in contact with thermostat with bosonic excitations. Exactly-solvable model.

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The relaxation of the harmonical oscillator, being in contact with the thermostat whose excitations can be treated as bosons is studied. Temperatures of the oscillator and thermostat are supposed to be different at  $t=0$ . An exact temporary behavior of the inverse oscillator's temperature is obtained. In low interaction limit the temperature behavior is exponential. When the interaction is increasing the temporary behavior display oscillations. *Narrow peak of the oscillator susceptibility is discovered.* The exact solution obtained is compared with Bloch-Redfield approximation.

## I. THE PROBLEM DESCRIPTION AND RESULTS

*If the reader knows some publications related to the susceptibility peak described below, please, send me the corresponding reference.*

The problems of kinetics are known to be one of the most complicated problems of physics. Existing approximate methods usually do not allow one to estimate the quality of the approximation, and the plausibility of the results is the main criteria of the validity of the approximation made. For this reason the simple exact-solvable models of dynamical system and thermostat are of particular interest. The exact solution can be compared in details with the solution, obtained by means of the approximate method. This allow one to evaluate used approximation in a correct way. Moreover the exact solution can demonstrate some new unexpected phenomena. We consider the resonance of the susceptibility described below to be one of them. In this paper we describe the model of this kind with the harmonical oscillator as a dynamical system and system having boson-like excitations as a thermostat. This model was considered by Bogolubov [1] for classical vibrator. The typical example of such thermostat is the phonon system of the crystal. The model's Hamiltonian in frequency units has form:

$$\begin{aligned}
 H &= H_p + H_s + H_{sp} \\
 H_p &= \sum_{q=1}^N \omega_q A_q^+ A_q, & H_s &= \omega_s B^+ B \\
 H_{sp} &= C_0 \sum_{q=1}^N (A_q B^+ + A_q^+ B), & C_0 &= \frac{b}{\sqrt{N}}
 \end{aligned} \tag{1}$$

Here  $H_p$  – the Hamiltonian of the bosonic thermostat,  $\omega_q$  – the boson's dispersion (for the phonon thermostat – the phonon frequencies)  $H_s$  – The Hamiltonian of the harmonical

oscillator,  $H_{sp}$  – the Hamiltonian of the interaction,  $N$  – number of bosonic modes,  $C_0$  – the interaction constant. The inverse proportionality of this constant to the number of bosonic modes  $N$  is typical for all known interactions.  $A_q^+, A_q(B^+, B)$  – the operators of creation and annihilation of bosones in  $q$ -mode (oscillator's energy quanta). The following commutation rules are taking place:

$$[A_q, A_{q'}^+] = \delta_{q,q'}, \quad [B, B^+] = 1 \quad (2)$$

We accept the simplest form for the bosonic spectrum:

$$\omega_q = \omega_s + \frac{2W}{N}(q - N/2 - 3/4), \quad q = 1, \dots, N \quad (3)$$

So, the oscillator frequency is coincide with bosones spectrum center. Suppose the oscillator and thermostat has at  $t = 0$  the temperatures  $T_{p0}$  and  $T_{s0}$  respectively. So, the problem is to solve the Lioville equation for the density matrix  $\rho$ :

$$i\dot{\rho} = [H, \rho] \quad (4)$$

with the initial condition:

$$\rho(0) = Z^{-1} \exp \left( -\frac{H_p + H_{sp}}{T_{p0}} - \frac{H_s}{T_{s0}} \right), \quad (5)$$

where

$$Z = \text{Sp} \exp \left( -\frac{H_p + H_{sp}}{T_{p0}} - \frac{H_s}{T_{s0}} \right) \quad (6)$$

Here we consider the temperature of interaction equal to that of thermostat. The unequilibrium state of this type can be obtained in a following way. Let the oscillator's frequency depends linearly on some external parameter  $h$ :  $\omega_s = \bar{\omega}h$ . Let this parameter has the value  $h'$  for a long time and our system reached the equilibrium, having the density matrix:  $\sim \exp -[\omega'_s B^+ B + H_{sp} + H_p]/T_{p0}$ ,  $\omega'_s = \bar{\omega}h'$ . Now let this parameter change instantaneously:  $h' \rightarrow h$ , and  $h - h' = \delta h$  and, therefore,  $\omega'_s \rightarrow \omega_s$ . After that the Hamiltonian of the system has the form (1). It is easy to see that right after jump of the parameter  $h$ , the density matrix can be represented in the form (5), with  $T_{s0} = (\omega_s/\omega'_s)T_{p0}$ . Thermostat is supposed to be microscopic, so all calculations below we perform in thermodynamic limit  $N \rightarrow \infty$ . Lastly note that the above model can describe the spin relaxation at temperatures low enough as compared with spin levels splitting in magnetic field. In this case the parameter  $h$  can be associated with magnetic field.

Thus problem is described, we now itemize the main points of the solution. For this reason we make the following general remark. Consider the set of operators  $O_i$ ,  $i = 1, \dots, M$  to be closed with respect to the commutation with Hamiltonian in the following sense:

$$[H, O_i] = \sum_{k=1}^M \alpha_{ik} O_k, \quad (7)$$

where  $\alpha_{ik}$  - numbers. Take now the density matrix in the form:

$$\sigma(t) = \sum_{i=1}^M \beta_i(t) O_i, \quad (8)$$

substitute it in (4). Making use of (7), we calculate commutators and equalize the factors corresponding to the similar operators. We obtain the following set of equations for  $\beta_i(t)$  functions:

$$\imath \dot{\beta}_i = \sum_{k=1}^M \beta_k \alpha_{ki}, \quad i = 1, \dots, M \quad (9)$$

After solving this set of equations we obtain the solution of Liouville equation in the form (8). Note now that the set of operators  $A_q^+ A_q$ ,  $A_q B^+$ ,  $A_q^+ B$ ,  $q = 1, \dots, N$  and  $BB^+$  is closed in the above sense with respect to the commutation with Hamiltonian (1) and we can use the above method as follows. Let us put into consideration the auxiliary density matrix  $\sigma$ :

$$\sigma = \sum_{q=1}^N \left( \beta_q A_q^+ A_q + \gamma_q A_q B^+ + \gamma_q^* A_q^+ B \right) + \beta_s B^+ B \quad (10)$$

Substituting it in (4) and equalizing the factors corresponding to the similar operators we obtain the following set of equations:

$$\begin{aligned} \imath \dot{\beta}_q &= C_0(\gamma_q - \gamma_q^*) \\ \imath \dot{\beta}_s &= -C_0 \sum_{q=1}^N (\gamma_q - \gamma_q^*) \\ \imath \dot{\gamma}_q &= (\omega_s - \omega_q) \gamma_q + C_0(\beta_q - \beta_s) \\ \imath \dot{\gamma}_q^* &= -(\omega_s - \omega_q) \gamma_q^* - C_0(\beta_q - \beta_s) \end{aligned} \quad (11)$$

We solve this system with initial conditions:

$$\beta_q(0) = \omega_q/T_{p0}, \quad \beta_s(0) = \omega_s/T_{s0}, \quad \gamma_q(0) = \gamma_q^*(0) = C_0/T_{p0} \quad (12)$$

After that we use known property of Liouville equation [2] (p. 170) : if matrix  $\sigma$  satisfy the Liouville's equation, then the arbitrary analitical function of this matrix satisfy the Liouville's equation too. Taking this into account, it is easy to see that matrix  $\rho = Z^{-1} \exp(-\sigma)$  satisfy the Liouville's equation with desired initial conditions (5). The final solution of the problem we obtain by turning to the thermodynamic limit  $N \rightarrow \infty$ . It is seen that functions  $\beta_q, \beta_s$  can be called the "dimensionless inverse temperatures" of the  $q$  bosonic mode and dynamical system respectively. We call  $\gamma_q$  functions the "dimensionless inverse temperatures of the interaction" with the bosonic mode  $q$ . An exact solution of (11) performed in the second section lead to the following formula for the temporary dependance of the inverse temperature of the oscillator  $T_s^{-1} = \beta_s(t)/\omega_s$  :

$$\frac{1}{T_s}(t) = \frac{1}{T_{s0}} + \left( \frac{1}{T_{p0}} - \frac{1}{T_{s0}} \right) \frac{2\tau}{\pi} \int_0^W \frac{1 - \cos \Omega t}{1 + \left( \Omega\tau - \Delta(\Omega) \right)^2} d\Omega \quad (13)$$

$$\tau^{-1} = \frac{\pi b^2}{W} = 2\pi b^2 \rho_0 \quad (14)$$

$$\Delta(\Omega) = \frac{1}{\pi} \ln \frac{W + \Omega}{W - \Omega} \quad (15)$$

Here  $\rho_0 \equiv 1/2W$  - is normalised to unit density of bosons modes. If  $b/W \ll 1$  one can extend the integration up to the infinity and drop the logarithmic term  $\Delta(\Omega)$  in denominator. After that the integral can be calculated and we obtain:

$$\frac{1}{T_s}(t) = \frac{1}{T_{s0}} + \left( \frac{1}{T_{p0}} - \frac{1}{T_{s0}} \right) \left( 1 - \exp - \left| \frac{t}{\tau} \right| \right) \quad (16)$$

The temporary dependences, calculated by formula (13) for different  $b/W$ , are presented on fig.1. It is seen that when interaction is small enough, the kinetics is exponential. Increasing of the interaction is accompanied by occurrence of oscillatory kinetics. We present here the expression for the inverse temperature of the bosonic q- mode  $q$   $1/T_q = \beta_q/\omega_q$ :

$$\frac{1}{T_q} = \frac{1}{T_{p0}} - \quad (17)$$

$$\left( \frac{1}{T_{p0}} - \frac{1}{T_{s0}} \right) \left( \frac{2b^2\omega_s\tau}{N\omega_q} \right) \left( \frac{2}{\pi} \int_0^W \frac{(1 - \cos \Omega t) d\Omega}{(\Omega^2 - \omega^2)[1 + (\Omega\tau - \Delta(\Omega))^2]} + (1 - \cos \omega t) \frac{\tau - \Delta(\omega)/\omega}{1 + (\omega\tau - \Delta(\omega))^2} \right)$$

$$\omega^2 \equiv (\omega_q - \omega_s)^2 + 2C_0^2$$

If  $b/W \ll 1$  this expression can be simplified:

$$\frac{1}{T_q} = \frac{1}{T_{p0}} - \quad (18)$$

$$\left( \frac{1}{T_{p0}} - \frac{1}{T_{s0}} \right) \left[ \frac{2b^2\tau\omega_s}{N\omega_q(1 + \omega^2\tau^2)} \right] \left[ \tau(1 - \cos \omega t) + \frac{\sin \omega |t|}{\omega} - \tau \left( 1 - \exp - \left| \frac{t}{\tau} \right| \right) \right]$$

Formula (14) can be rewritten in the form:

$$\tau^{-1} = 2\pi b \rho_0(\omega_s) \quad (19)$$

$\rho_0(\omega_s)$  - density of the resonance bosonic modes.

Let us now return to the dropped logarithmic term which can be of particular interest for the following reason. The above problem describes the 'system's response' on the jump of the parameter  $h$ . If we consider the 'system's response' as  $\delta(1/T_s) \equiv (1/T_s - 1/T_{p0})$ , then  $\delta(1/T_s) = \Phi(t)\delta h$ , where  $\Phi(t)$  can be derived from (13). Let parameter  $h$  gains small

harmonical increment  $\delta h_\omega \exp i\omega t$ . The corresponding small modulation  $\delta(1/T_s)_\omega \exp i\omega t$  can be expressed in terms of susceptibility:

$$\delta\left(\frac{1}{T_s}\right)_\omega = \chi_\omega \delta h_\omega$$

On the other hand, the linear response theory [2] (. 88) lead to the following relationship between the susceptibility and 'system's response' on the jump  $\Phi(t)$ :

$$\Phi(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{\chi_\omega e^{i\omega t}}{i\omega + 0} d\omega, \quad \chi_\omega = i\omega \int_0^{+\infty} e^{-i\omega t} \Phi(t) dt$$

The imaginary part of susceptibility can be explicitly calculated. It differs from zero only when  $-W < \omega < W$  and is equal to:

$$\text{Im } \chi_\omega = \chi_\infty \frac{\omega\tau}{1 + (\omega\tau - \Delta(\omega))^2} \quad \chi_\infty \equiv -\frac{\bar{\omega}_s}{T_{p0} \omega_s}$$

It is seen that susceptibility  $\text{Im } \chi_\omega$  exhibit two extraordinary extremums whose positions  $\pm\omega_0$  (when  $b/W \ll 1$ ) can be defined from the equation:

$$\omega_0\tau = \Delta(\omega_0)$$

It is easy to see that  $\omega_0 \approx W - 0$ . So, if  $\omega = \omega_0$  the modulation of oscillator's inverse temperature in the orthogonal phase (with respect to  $\delta h$ ), is  $W\tau = (W/b)^2/\pi \gg 1$  times greater than the adiabatic modulation  $\chi_\infty \delta h$ . If interaction is small enough, it is possible to estimate the absorption under the action of modulation  $\delta h = \delta h_\omega \sin \omega t$ . The rate of energy changing  $dE/dt$  for whole system (oscillator+thermostat) can be calculated as:

$$\frac{dE}{dt} = \frac{d}{dt} \text{Sp } \rho H = \text{Sp } \rho \frac{d}{dt} H_s = \bar{\omega}_s \dot{\delta h} \text{Sp } \rho B^+ B = \bar{\omega}_s \dot{\delta h} < n >$$

If the interaction is small, terms  $\sim \gamma_q$  can be omitted in  $\rho \sim \exp(-\sigma)$ . In this case the average number of quanta  $< n >$  is defined by the Bose-Einstein function  $< n > = 1/(e^{\beta_s} - 1)$  with  $\beta_s = \omega_s/T_s$  depending on time. Linear response  $\delta\beta_s$  related to the modulation  $\delta h$  can be determined by above expression for susceptibility. Furthermore  $dE/dt$  should be averaged over the period of oscillations. For this reason only the component of  $\delta(1/T_s)$  having the same phase as  $\dot{\delta h}$  is important. It is defined by above expression for the imaginary part of the susceptibility. Taking all this into account it is easy to see that  $\langle dE/dt \rangle$  is differs from zero only if  $0 < \omega < W$  and in this frequency interval can be calculated as:

$$\left\langle \frac{dE}{dt} \right\rangle = \frac{\delta\omega_s^2}{2T_{p0}} \frac{e^\beta}{(e^\beta - 1)^2} \frac{\omega^2\tau}{1 + [\omega\tau - \Delta(\omega)]^2} \quad \beta \equiv \frac{\omega_s}{T_{p0}}, \quad \delta\omega_s \equiv \bar{\omega}_s \delta h_\omega$$

The frequency behaviour of the absorption is presented diagrammatically on fig.1 (c). It is seen that the absorption exhibit narrow maximum at  $\omega = \omega_0$ . The occurrence of this maximum is somewhat unexpected. This peak do not depend on details of the bosonic spectrum.

## II. THE EQUATION FOR THE INVERSE TEMPERATURES

In this section we solve the set of equations (11) which can be rewritten as:

$$\ddot{I}_q = -[(\omega_q - \omega_s)^2 + 2C_0^2]I_q - 2C_0^2 \sum_{q'=1}^N I_{q'} \quad q = 1, \dots, N \quad (20)$$

$$I_q \equiv \gamma_q^* - \gamma_q$$

As a starting point we find the solutions of this equation having the harmonical temporary dependance - normal modes  $e_q^\Omega \exp(i\Omega t)$ ,  $q = 1, \dots, N$ .

After substituting in (20) we obtain the following equations for the amplitudes  $e_q^\Omega$ :

$$e_q^\Omega = -\frac{2C_0^2 S}{(\omega_s - \omega_q)^2 + 2C_0^2 - \Omega^2} \quad q = 1, \dots, N \quad (21)$$

where

$$S \equiv \sum_{q=1}^N e_q^\Omega \quad (22)$$

Substituting (21) in (22) we obtain for squares of eigen frequencies  $\Omega^2$ :

$$\sum_{q=1}^N \frac{2C_0^2}{(\omega_s - \omega_q)^2 + 2C_0^2 - \Omega^2} = -1 \quad (23)$$

For the bosonic spectrum in the form (3) this equation have  $N$  undegenerated roots. Using (21) we obtain for the normal modes the following expression:

$$e_q^\Omega = \frac{N_0(\Omega)}{(\omega_s - \omega_q)^2 + 2C_0^2 - \Omega^2} \quad (24)$$

Where  $N_0(\Omega)$  is defined as:

$$N_0^{-2}(\Omega) = \sum_{q=1}^N \left[ \frac{1}{(\omega_s - \omega_q)^2 + 2C_0^2 - \Omega^2} \right]^2 \quad (25)$$

(24) is the eigen mode of (20) only if  $\Omega^2$  is coincide with one of the roots of (23). The initial conditions for quantities  $I_q$  can be obtained from (12):

$$I_q(0) = 0, \quad \dot{I}_q(0) = 2iC_0\omega_s \left( \frac{1}{T_{p0}} - \frac{1}{T_{s0}} \right) \quad (26)$$

Introducing the solution of (20) in the form of expansion over the normal modes, we can write down the solution of (20) as:

$$I_q(t) = 2iC_0\omega_s \left( \frac{1}{T_{p0}} - \frac{1}{T_{s0}} \right) \sum_{q'} \frac{e_q^\Omega e_{q'}^\Omega \sin \Omega t}{\Omega} \quad (27)$$

$\Omega$  runs over the set of eigen frequencies obtained from (23). From (23) and (24) one can obtain:

$$\sum_q e_q^\Omega = -\frac{N_0(\Omega)}{2C_0^2} \quad (28)$$

Using this relationship we obtain the solution of (20) in the form:

$$I_q = -i\frac{\omega_s}{C_0}\left(\frac{1}{T_{p0}} - \frac{1}{T_{s0}}\right) \sum_\Omega \frac{N_0^2(\Omega) \sin \Omega t}{\Omega [(\omega_q - \omega_s)^2 + 2C_0^2 - \Omega^2]} \quad (29)$$

Taking into account (28), (27), (11) and initial conditions for  $1/T_s = \beta_s/\omega_s$  it is easy to obtain:

$$\left(\frac{1}{T_s}\right) = \left(\frac{1}{T_{s0}}\right) + \frac{1}{2C_0^2}\left(\frac{1}{T_{p0}} - \frac{1}{T_{s0}}\right) \sum_\Omega N_0^2(\Omega) \frac{1 - \cos \Omega t}{\Omega^2} \quad (30)$$

The sum in this formula can be replaced by integral if density of squares of eigen frequencies  $\Omega^2$  is known. We calculate this density as follows. The above eigen frequencies arises in the following problem for eigen values:  $\hat{M}\mathbf{e} = \Omega^2\mathbf{e}$ , where matrix  $\hat{M}$  is defined as:

$$\hat{M} = \hat{M}_0 + \hat{V} \quad (31)$$

$$\hat{M}_0 = \begin{pmatrix} d_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & d_N \end{pmatrix} \quad \hat{V} = 2C_0^2 \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix}$$

$$d_m = (\omega_s - \omega_q)^2 + 2C_0^2 \rightarrow \frac{W^2}{N^2}(m + 1/2)^2 + 2C_0^2$$

The diagonal elements  $d_m$  are written for the bosonic spectrum in the form (3). Let us put into consideration the Green's function:

$$\hat{G}(E) = (E - \hat{M})^{-1} \quad (32)$$

Then the density of squares of eigen frequencies of interest  $D(\Omega^2)$  is defined by known formula:

$$D(E) = -\frac{1}{\pi} \text{Im Sp } \hat{G}(E), \quad E = \Omega^2 + i\delta \quad \delta \rightarrow +0 \quad (33)$$

Considering  $\hat{V}$  as perturbation for  $\hat{M}_0$ , one can write down the Dyson's expansion for Green's function:

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G}_0 + \hat{G}_0\hat{V}\hat{G}_0\hat{V}\hat{G}_0 + \dots \quad \hat{G}_0 \equiv (E - \hat{M}_0)^{-1} \quad (34)$$

This series can be exactly summed and for the  $\text{Sp } \hat{G}$  of interest we obtain:

$$\text{Sp } \hat{G}(E) = \frac{\Gamma(E)}{2C_0^2} - \frac{\partial \Gamma / \partial E}{1 - \Gamma(E)} \quad (35)$$

where

$$\Gamma(E) \equiv 2C_0^2 \sum_m \frac{1}{E - d_m} = 2C_0^2 \text{Sp } \hat{G}_0 \quad (36)$$

For the bosonic spectrum in the form (3) in the thermodynamic limit one can write down the explicit expression for  $\Gamma(E)$ :

$$\begin{aligned} \Gamma(E) &= \left(\frac{2b^2}{N}\right) \sum_{m=0}^N \frac{1}{E - (W/N)^2(m + 1/2)^2 - 2b^2/N} = \\ &= 2b^2 \int_0^1 \frac{d\xi}{E - (W\xi)^2} = \frac{b^2}{W\sqrt{E}} \ln \frac{\sqrt{E} + W}{\sqrt{E} - W} \end{aligned} \quad (37)$$

Factor (25) can be presented in terms of  $\Gamma(E)$  as:

$$N_0^2(\Omega) = -\frac{2C_0^2}{\partial\Gamma/\partial E} \quad E = \Omega^2 \quad (38)$$

And taking into account (33), (35) we obtain the following relationship:

$$\frac{1}{2C_0^2} \sum_{\Omega} \frac{N_0^2(\Omega)}{\Omega^2} (1 - \cos \Omega t) = -\frac{1}{\pi} \text{Im} \int \frac{dE}{1 - \Gamma(E)} \frac{1 - \cos \sqrt{E}t}{E} \quad (39)$$

Making use of (30), (39) it is now easy to obtain (13). Formula (17) can be obtained in the same manner.

### III. THE COMPARISON WITH BLOCH-REDFIELD'S THEORY.

This theory [2] (. 60) lead to the following kinetic equation for the diagonal elements of density matrix of above oscillator:

$$\dot{\rho}_n = \rho_{n+1}W_{n+1 \rightarrow n} + \rho_{n-1}W_{n-1 \rightarrow n} - \rho_n(W_{n \rightarrow n+1} + W_{n \rightarrow n-1}) \quad (40)$$

where  $W_{n \rightarrow n \pm 1}$  :

$$W_{n \rightarrow n+1} = \frac{1}{\tau} \frac{n+1}{\exp(\omega_s/T_{p0}) - 1} \quad (41)$$

$$W_{n+1 \rightarrow n} = W_{n \rightarrow n+1} \exp(\omega_s/T_{p0})$$

With  $\tau$  determined by formula (14). It is seen that the temporary behaviour of density matrix in Bloch-Redfield approximation do not agreed with above exact solution. But the relaxation time of the average energy of the oscillator  $\langle n \rangle = \sum_n \rho_n n$  is coincide with (14) This can be shown by multiplying (40) by  $n$  and summing over all states:

$$\langle \dot{n} \rangle = \frac{1}{\tau} \left[ \frac{1}{\exp(\omega_s/T_{p0}) - 1} - \langle n \rangle \right] \quad (42)$$



- [1] N.N.Bogolubov, Selected transactionses, Naukova Dumka, Kiev 1970.
- [2] I.V.Alexandrov, *The theory of magnetic relaxation*, .: Nauka, 1975.

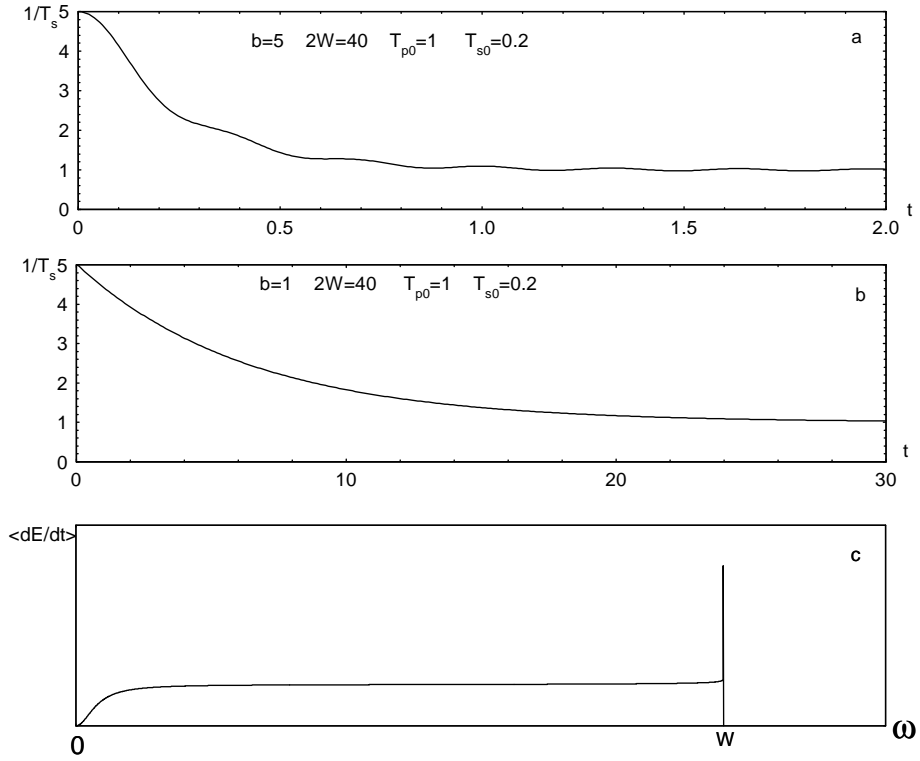


FIG. 1. The kinetics of the inverse temperature of the oscillator for various strength of interaction (a,b). The frequency dependance of absorption (c).